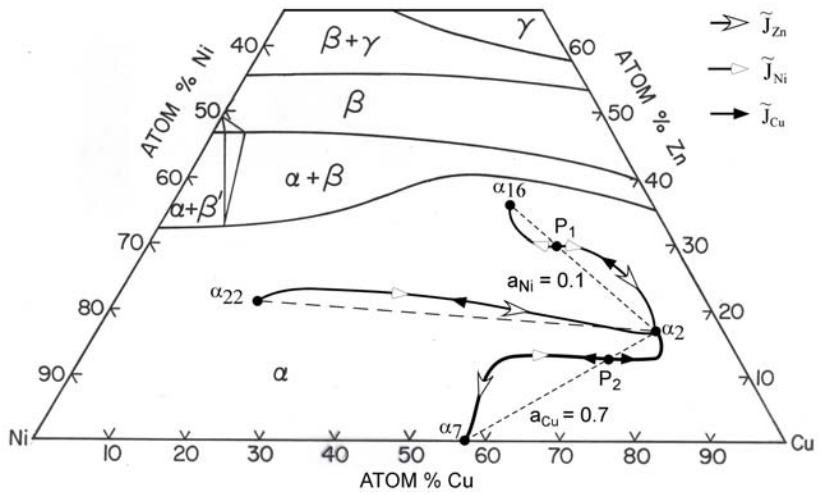
Zero-Flux Planes in Multicomponent Systems and Development of *Multi*DiFlux Program - Version 1.2

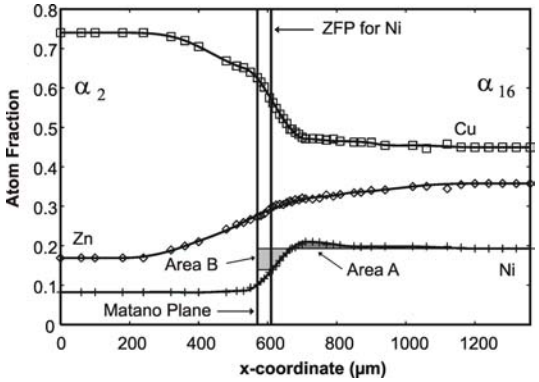
M.A. Dayananda, Purdue University —DMR-0304777

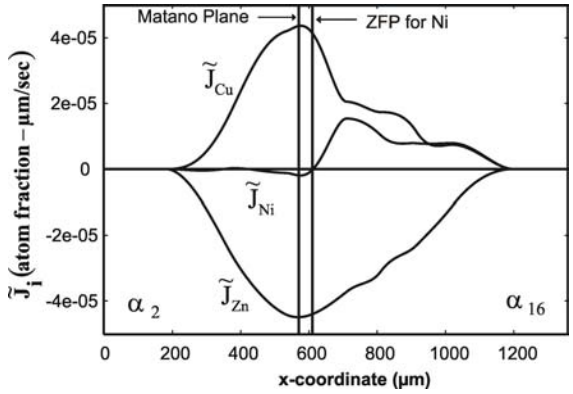
Motivation and Experiments

Interdiffusion in multicomponent systems can give rise to the development of zero-flux planes (ZFP), where the flux of a component goes to zero within the diffusion zone and exhibits a change in flux direction from one side of the ZFP to the other. Controlled development of ZFPs can help control interdiffusion of a component. Diffusion experiments have been carried out for ZFP development with several Cu-Ni-Zn diffusion couples annealed at 775°C. ZFP compositions (P_1 and P_2) developed for selected couples are shown on the diffusion paths below. Directions of interdiffusion fluxes $\tilde{J}_i$ of the individual components are also identified on either side of the ZFPs.

A user-friendly computer program called *Multi*DiFlux (version 1.2) was developed and applied to the analysis of the diffusion couples for the determination of interdiffusion fluxes of all components, identification of ZFPs and the ternary interdiffusion coefficients as functions of composition. An application of the program to a couple is shown below.







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Broad Impact

Two invited talks were presented in a NIST workshop held in April 2004 on interdiffusion microstructures in multicomponent systems and the application of *Multi*DiFlux program (version 1.2) to multicomponent diffusion analysis. The program can be down-loaded as a free educational and research tool for diffusion studies of single phase systems at the site: https://engineering.purdue.edu/MSE/Fac Staff/Faculty/dayananda.wshtml

A technical paper on the use of *Multi*DiFlux program will be presented at the Materials Science and Technology meeting to be held in New Orleans in September 25-29, 2004.

An invited, technical article entitled "Interdiffusion Structures" by J. E. Morral and M. A. Dayananda, is *in print* in Metals Handbook, Vol.9, ASM, New Edition (2004)

Education

There are two graduate students associated with the project. Kevin M. Day, a Ph.D student, has investigated several Cu-Ni-Zn diffusion couples for the development of zero-flux planes. He has also analyzed them with *Multi*DiFlux program for ternary interdiffusion coefficients. Kaustubh N. Kulkarni, a M.S. student, is investigating isoactivity diffusion couples that can develop multiple zero-flux planes to control diffusion of a component. Dr. L. Ram-Mohan of Quantum Semiconductor Algorithms has been an active consultant and contributor to the development of the computer code.